

Hexachloroethane
67-72-1 | DTXSID7020689

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 452

Global applicability domain: Inside

Local applicability domain index: 5.87e-01

Confidence level: 5.91e-01

Nearest Neighbors from the Training Set

Image not found

Hexachloroethane

Measured: 513

Predicted: 452

Image not found

Hexachloro-1,3-butadiene

Measured: 6610

Predicted: 3610

Image not found

Carbon tetrachloride

Measured: 7.41

Predicted: 12.9

Image not found

Tetrachloroethylene

Measured: 52.5

Predicted: 42.2